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2D carbon allotropes under confinement

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ABSTRACT

Graphene is not the only carbon-based 2D material of recent interest; a class of materials called “graphynes” have been making an impact for their promising properties as well [1-3]. Graphynes are similar to graphene in that they are planar networks of carbon atoms, and many of them have lattices with hexagonal symmetry. Unlike graphene however, graphynes are composed of both sp2- and sp3-hybridized carbons. This gives graphynes a whole slew of properties not found in pristine graphene, allowing for unique chemical functionalization and tunable electronic attribute. In much the same way as crumpling a piece of paper transforms a sheet-like material into a three-dimensional object with relatively high compressive strength while maintaining a large surface area and free volume, the same mechanism occurs when crumpling planar nanomaterials such as graphene and its derivatives [4-6]. The potentiality of crumpling as a method to tailor the properties of graphene and graphene oxide while maintaining surface area has been explored in earlier studies [6-12], but to the authors’ knowledge this report is the first to make a cohesive study on the crumpling behavior of graphynes. In this study, we systematically examine the behavior of graphynes under geometric confinement across various temperatures, sizes, and crumpling rates, and compare them to graphene under the same conditions. The sp3-hybridized carbons in graphynes are more potentially reactive than the carbons in graphene; as such the graphynes exhibit a markedly increased affinity for interlayer attraction. It is shown that the 2D carbon materials tested here show similar behaviors across many conditions, with the most important behavior-determining factor being the number of linking sp3-hybridized carbons in the material.

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